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Note

Hypergraphs and the Clar problem in hexagonal systems

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Abstract

We show that for a hypergraph H that is separable and has the Helly property, the perfect matchings of H are the strongly stable sets of the line graph of H. Also, we show that the hypergraph generated by a hexagonal system is separable and has the Helly property. Finally, we note that the Clar problem of a hexagonal system is a minimum cardinality perfect matching problem of the hypergraph generated by the hexagonal system. Hence, the Clar problem of a hexagonal system is a minimum cardinality strongly stable set problem in the line graph of the hypergraph generated by the hexagonal system.

Keywords: Separable hypergraph; Helly property; Hexagonal system; Resonant set

1. Introduction

A hexagon is *regular* if all its edges are equal and all its angles are equal. Two regular hexagons are *congruent* if their edges are equal. The plane can be completely covered by congruent regular hexagons and the infinite plane graph formed is called the *hexagonal lattice*. Let us note here that our graphs are finite unless otherwise stated. A *hexagonal system* is a 2-connected subgraph of the hexagonal lattice without non-hexagonal interior faces. Hexagonal systems are used to represent the molecules of chemical compounds known as benzenoid hydrocarbons. The mathematical theory of hexagonal systems and its relevance to chemistry are presented in [1,2].

An interesting optimization problem in hexagonal systems is the so-called Clar problem that is defined as follows. Let P be a non-empty set of hexagons of a hexagonal system H. We call P a *resonant set* of H if the hexagons in P are pair-wise disjoint and the subgraph of H obtained by deleting from H the vertices of the hexagons in P has a perfect matching or is empty [3,4]. Alternatively [5], P is a resonant set if the hexagons in P are pair-wise disjoint and there exists a perfect matching of H that contains a perfect matching of each hexagon in P. A resonant set is *maximum* if its cardinality is maximal among all the resonant sets. The cardinality of a maximum resonant set is called the *Clar number* [6] since it was Clar [7] who noticed its significance in chemistry. It was shown [8] that a hexagonal system has a resonant set if and only if it has a perfect matching. By solving the *Clar problem* in a hexagonal system that has a perfect matching, we mean obtaining a maximum resonant set and computing its cardinality, the Clar number. The Clar problem was studied in [5,6,9–12]. In particular, Abeledo and Atkinson [5,9] showed that the Clar problem could

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be solved in polynomial time as a linear program. Polynomial combinatorial algorithms to solve the Clar problem for special classes of hexagonal systems were studied in [9,13–15]. However, it is still an open problem to design a polynomial combinatorial algorithm to solve the Clar problem in the general case.

Certain polynomials that are related to the Clar problem have been introduced and studied. These are the sextet polynomial [3,16–20], the cell polynomial [21,18], a generalization of the sextet polynomial, and the Clar covering polynomial [22,23].

The main chemical implication of the Clar number is the following empirically established regularity [7]: If B_a and B_b are two isomeric benzenoid hydrocarbons, and if the Clar number of B_a is greater than the Clar number of B_b, then the compound B_a is both chemically and thermodynamically more stable. Also, Aihara [24] noted that when a benzenoid hydrocarbon has a unique maximum resonant set, the hexagons of the set specify the locations where the resonance energy is densely distributed. Recently, Gutman et al. [25] showed a relation between the Clar covering polynomial of a benzenoid hydrocarbon and the resonance energy.

In Section 3 of this paper, we prove a result on the perfect matchings of a class of hypergraphs. In Section 4, we show that this result is applicable to the hypergraph generated by a hexagonal system, allowing a new mathematical interpretation of the Clar problem in hexagonal systems. We begin by providing in Section 2 some background material on graphs and hypergraphs.

2. Preliminaries on graphs and hypergraphs

Introductory material on graphs and hypergraphs can be found in [26–28].

A *clique* of a graph is a non-empty set of vertices that are pair-wise adjacent. A clique is *maximal* if it is not contained in another clique. The *clique matrix* [29] of a graph G is a 0, 1 matrix whose columns are indexed by the vertices of G and whose rows are the incidence vectors of the maximal cliques of G. A *stable* or *independent set* of a graph is a non-empty set of vertices, no two of which are adjacent. A *strongly stable set* [30] of a graph G is a stable set of G which intersects every maximal clique of G.

A graph is said to be *embedded* in the plane if it is drawn in the plane so that no two edges intersect. A graph is *planar* if it can be embedded in the plane. A *plane* graph is a planar graph together with a particular embedding in the plane. We call the regions of the plane defined by a plane graph *faces*, the unbounded region being called the *exterior* or *infinite* face and the other bounded regions, if any, are called *interior* or *finite* faces. If the boundary of a face of a plane graph is a cycle, we sometimes refer to the cycle or its vertex set as a face. The meaning will be evident from context. In a 2-connected plane graph, every face boundary is a cycle.

Let X be a finite non-empty set. A *hypergraph* on X is a non-empty family H of non-empty subsets of X whose union is X. The elements of X are called the *vertices* and the sets in H are the *edges* of the hypergraph. The (*vertex-edge*) *incidence matrix* of a hypergraph H is a 0,1 matrix with rows indexed by the vertices of H and whose columns are the incidence vectors of the edges of H.

Let H be a hypergraph. An *intersecting family* of H is a non-empty family of edges having non-empty pair-wise intersection. For example, for every vertex x of H, $H(x) = \{E | E \in H \text{ and } x \in E\}$, called the *star with center* x, is an intersecting family of H. We say that a hypergraph H has the *Helly property* if every intersecting family of H has a non-empty intersection. A hypergraph is *separable* if for every vertex x, the intersection of the edges in $H(x)$ is the singleton $\{x\}$. A *matching* in a hypergraph is a non-empty family of pair-wise disjoint edges. A matching M in a hypergraph is *perfect* if every vertex belongs to some edge in M.

Given a hypergraph H, its *line graph* $L(H)$, also called *intersection graph*, is the graph whose vertices are the edges of H and two vertices are adjacent if they have a non-empty intersection.

Let G be a 2-connected plane graph with vertex set V, edge set E and set of interior faces F. Here, a face refers to the vertex set of its boundary. It is clear that $E \cup F$ is a hypergraph on V [9] and we call it the *hypergraph generated by* G. To avoid confusion, we call the edges of this hypergraph *hyperedges*.

3. Perfect matchings in separable hypergraphs with the Helly property

The following lemma shows that for a hypergraph H that is separable and has the Helly property, there exists a bijective mapping of the vertex set of H into the family of maximal cliques of $L(H)$. It also establishes that the incidence matrix of a separable hypergraph H with the Helly property is the clique matrix of its line graph $L(H)$. The relationship between hypergraphs and line graphs was explored by Gilmore and Berge (see [31,28]). In particular, the lemma below can be shown to follow from their results, but it is simpler to provide a direct proof instead.

Lemma 3.1. *Let H be a hypergraph that is separable and has the Helly property. Then* (i) *for each vertex v of H, $H(v)$ is a maximal clique of $L(H)$,* (ii) *for distinct vertices u and v of H, $H(u)$ and $H(v)$ are also distinct, and* (iii) *a maximal clique of $L(H)$ is equal to $H(v)$ for some vertex v of H.*

Proof. Let v be a vertex of H. Since $H(v)$ is an intersecting family of H, $H(v)$ is a clique of $L(H)$. Assume that $H(v)$ is not a maximal clique of $L(H)$. Then there exists an edge E of H such that $E \notin H(v)$ and $\{E\} \cup H(v)$ is an intersecting family of H. Since H has the Helly property, $\{E\} \cup H(v)$ has a non-empty intersection. Also, the intersection of the edges in $\{E\} \cup H(v)$ is a subset of the intersection of the edges in $H(v)$. Since H is separable, the latter intersection is the singleton $\{v\}$. Hence, the intersection of the edges in $\{E\} \cup H(v)$ is the singleton $\{v\}$ and $E \in H(v)$, a contradiction.

For distinct vertices u and v of H, $H(u)$ and $H(v)$ are also distinct since H is separable.

Let S be a maximal clique of $L(H)$. Since S is a clique of $L(H)$, it is an intersecting family of H. Since H has the Helly property, the intersection of the edges in S is non-empty. Let v belongs to this intersection. Then $S \subset H(v)$. Since S is a maximal clique of $L(H)$ and $H(v)$ is a clique, $S = H(v)$. □

Theorem 3.2. *Let H be a hypergraph that is separable and has the Helly property. The perfect matchings of H are the strongly stable sets of the line graph of H.*

Proof. A strongly stable set of $L(H)$ is a stable set of $L(H)$. Hence, it is a matching of H. Let v be a vertex of H. By Lemma 3.1, $H(v)$ is a maximal clique of $L(H)$. The strongly stable set intersects this maximal clique $H(v)$. Hence, v belongs to an edge in the matching and so the matching is perfect.

A perfect matching of H is a matching of H. Hence, it is a stable set of $L(H)$. By Lemma 3.1, a maximal clique of $L(H)$ is equal to $H(v)$ for some vertex v of H. The vertex v belongs to some edge in the perfect matching. Hence, the stable set intersects the maximal clique and so it is a strongly stable set of $L(H)$. □

4. An application in hexagonal systems

In this section, we show that the hypergraph generated by a hexagonal system is separable and has the Helly property, thus Theorem 3.2 is applicable. This allows a new mathematical interpretation of the Clar problem as justified by the discussion towards the end of the section. We need the following characterization by Berge [32, 28] of hypergraphs that have the Helly property.

Proposition 4.1 (*[32,28]*). *A hypergraph has the Helly property if and only if for any three vertices a_1, a_2 and a_3, the family of the edges containing at least two of the vertices a_i is either empty or has a non-empty intersection.*

Theorem 4.2. *Let B be a hexagonal system. The hypergraph generated by B has the Helly property.*

Proof. We use Proposition 4.1. Let a_1, a_2 and a_3 be three vertices. Assume that the family of hyperedges containing at least two of the vertices a_i is non-empty. We show that this family has a non-empty intersection. The hyperedges in this family can be classified into the following types: (i) type-123: are hyperedges containing the three vertices, (ii) type-12: are hyperedges containing a_1 and a_2 but not a_3, (iii) type-13: are hyperedges containing a_1 and a_3 but not a_2, (iv) type-23: are hyperedges containing a_2 and a_3 but not a_1.

Case: The set $\{a_1, a_2, a_3\}$ is not a stable set of B. Hence, there exist two of the vertices a_i that are adjacent in B. Without loss of generality, we can assume that these two vertices are a_1 and a_2. *Subcase*: The vertices a_1 and a_3 are adjacent in B. The situation is depicted in Fig. 1 and it can be seen that type-23 hyperedges do not exist in the family. Hence, a_1 belongs to the intersection of the family and so the family has a non-empty intersection. *Subcase*: The vertices a_1 and a_3 are not adjacent in B. If type-13 hyperedges do not exist in the family then a_2 belongs to the intersection of the family and the family has a non-empty intersection. Otherwise, there exists a hexagon containing a_1 and a_3 but not a_2. The situation is depicted in Fig. 2 and it can be seen that type-23 hyperedges do not exist in the family. Hence, a_1 belongs to the intersection of the family and so the family has a non-empty intersection.

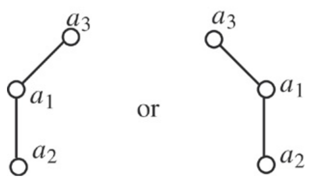

Fig. 1. The vertices a_1 and a_2 are adjacent and the vertices a_1 and a_3 are adjacent.

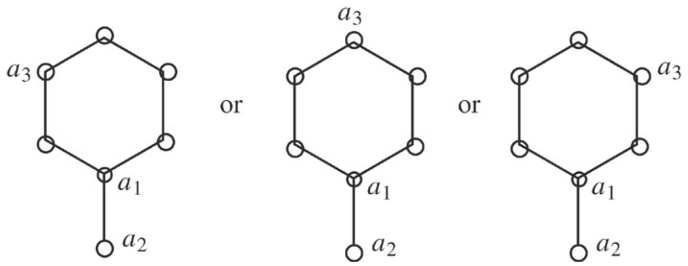

Fig. 2. The vertices a_1 and a_2 are adjacent, the vertices a_1 and a_3 are not adjacent and there exists a type-13 hyperedge in the family.

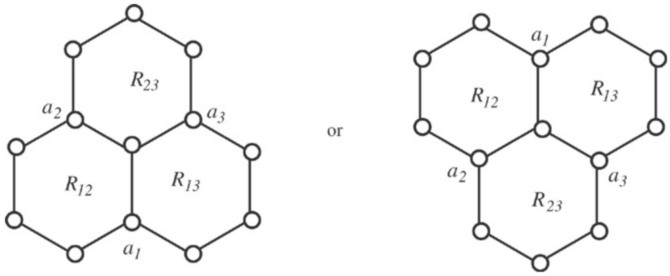

Fig. 3. $\{a_1, a_2, a_3\}$ is a stable set of B, and type-12, type-13 and type-23 hyperedges co-exist in the family.

Case: The set $\{a_1, a_2, a_3\}$ is a stable set of B. If type-12, type-13 and type-23 hyperedges do not co-exist in the family then the family has a non-empty intersection. Otherwise, type-12, type-13 and type-23 hyperedges co-exist in the family and it is clear that all these hyperedges are necessarily hexagons. Moreover, there exists exactly one hyperedge of each of these types in the family. Let us denote these hexagons by R_{12}, R_{13} and R_{23}. The situation is depicted in Fig. 3 and it can be seen that type-123 hyperedges do not exist in the family. Hence, the family is $\{R_{12}, R_{13}, R_{23}\}$. It can be seen from Fig. 3 that there exists a vertex that is common among R_{12}, R_{13}, R_{23} and so the family has a non-empty intersection. □

Proposition 4.3. *Let G be a 2-connected plane graph. The hypergraph generated by G is separable.*

Proof. Let v be a vertex. Since G is 2-connected, there exists more than one edge of G incident with v. Hence, the intersection of the edges of G containing v is the singleton $\{v\}$. Since the family of hyperedges containing v contains the family of edges of G containing v, the result follows. □

Theorem 4.4. *Let B be a hexagonal system. The perfect matchings of the hypergraph generated by B are the strongly stable sets of the line graph of the hypergraph generated by B.*

Proof. It follows from Theorems 3.2 and 4.2 and Proposition 4.3. □

Discussion

Consider a hexagonal system that has a perfect matching. Let $\boldsymbol{Q}$ be its vertex-edge incidence matrix and $\boldsymbol{R}$ its vertex-hexagon incidence matrix. Consider the following integer linear program (ILP)

$$\min\{\mathbf{1}^t\boldsymbol{x} + \mathbf{1}^t\boldsymbol{y} | \boldsymbol{Qx} + \boldsymbol{Ry} = \mathbf{1}; \boldsymbol{x}, \boldsymbol{y} \text{ binary}\}. \tag{1}$$

This ILP models the Clar problem [10,12]. In particular, it can be shown that there exists a 1–1 mapping of the set of optimal solutions of this ILP onto the family of maximum resonant sets of the hexagonal system, i.e. the mapping is bijective. The image of an optimal solution $(\,\boldsymbol{x}^t \quad \boldsymbol{y}^t\,)^t$ under this mapping is the set of hexagons corresponding to the 1's in $\boldsymbol{y}$. The constraint matrix $(\,\boldsymbol{Q} \quad \boldsymbol{R}\,)$ of this ILP is the vertex-hyperedge incidence matrix of the hypergraph generated by the hexagonal system [9]. Therefore, there exists a 1–1 mapping of the feasible solutions of this ILP onto the perfect matchings of the hypergraph generated by the hexagonal system [9]. The image of a feasible solution $(\,\boldsymbol{x}^t \quad \boldsymbol{y}^t\,)^t$ under this mapping is the set of hyperedges corresponding to the 1's in $(\,\boldsymbol{x}^t \quad \boldsymbol{y}^t\,)^t$. Hence, the Clar problem in a hexagonal system is a minimum cardinality perfect matching problem in the hypergraph generated by the hexagonal system. Theorem 4.4 admits an alternative interpretation stated in the following theorem.

Theorem 4.5. *The Clar problem in a hexagonal system is a minimum cardinality strongly stable set problem in the line graph of the hypergraph generated by the hexagonal system.*

Remark. It is worth mentioning that Gutman et al. [33] considered hexagonal systems with unique maximum resonant sets. For such a hexagonal system, they defined the so-called *Clar hypergraph*. Its vertex set is the vertex set of the hexagonal system and its edge set is the union of the edge set of the hexagonal system and the (unique) maximum resonant set of the hexagonal system.

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